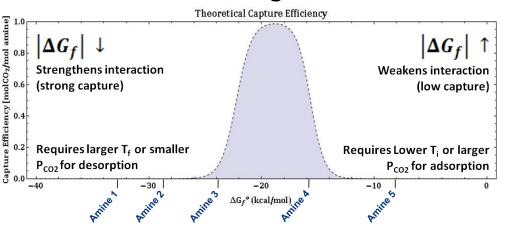
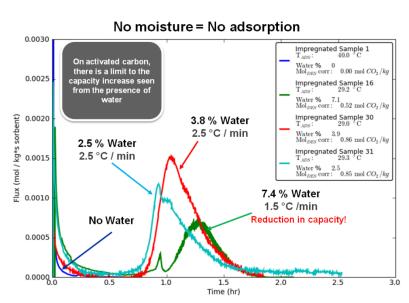
Good capture agents compromise capacity with ease of regeneration



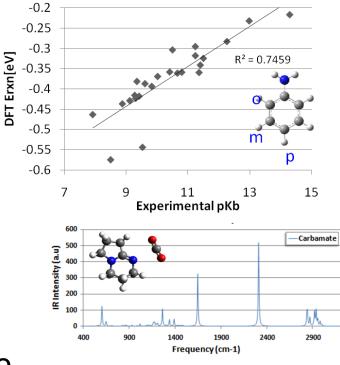
How do we identify the right amine for an application?

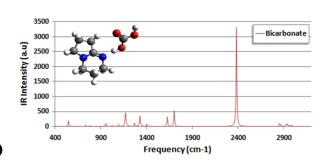
How do we quantitatively model the role of moisture and sorbent properties on capacity and regeneration?



What are the limits, and what are the constraints?

Computational approaches to screening reactivity and mechanism identification





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